

**METADATA AND NUMERICAL DATA CAPTURE:
Critical Temperature
(for 1 – Component)**

***Guided Data
Capture (GDC)***



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Critical Temperature (1 component)**
with the Guided Data Capture (GDC) software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. **It is not necessary to enter *all* compounds before entering *all* samples, etc.**

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

J. Chem. Eng. Data 2000, 45, 157–160

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Critical Point and Vapor Pressure Measurements at High Temperatures by Means of a New Apparatus with Ultralow Residence Times

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A new flow method has been employed to obtain critical point and vapor pressure data at high temperatures for four compounds: squalane, toluene, ethylbenzene, and styrene. This new flow method allows the determination of reliable critical points and vapor pressures for thermally unstable or otherwise reactive compounds. The critical point is inferred from other measurements in the critical region. The measurement accuracy is less than that obtained by more conventional methods, but this method has been used where conventional methods fail.

Critical Temperature for 1 component squalane

Table 1. Results of Critical Point Measurements

compound	T_c/K			P_c/MPa		
	meas	previous	est ^a	meas	previous	est ^a
squalane	795.9		882.5	0.59		0.83
toluene	591.8	591.90 ^b 591.79 ^c 591.75 ^d	598.4	4.11	4.111 ^b 4.109 ^c 4.108 ^d	4.13
ethylbenzene	618.0	617.26 ^b 617.20 ^c 617.15 ^d	623.3	3.62	3.616 ^b 3.606 ^c 3.609 ^d	3.66
styrene	635.2		644.1	3.87		3.86

This experimental value is
considered here.

Experimental Method Info :

Flow Method

Author's uncertainty estimates:

T_c : 1 K

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application. The menu bar includes 'File', 'Edit', 'Tools', and 'Help'. The main window has a tabbed interface with 'Reference', 'Compound', 'Sample', 'Mixture', 'Reaction', 'Property', and 'Data Tables'. The 'Property' tab is selected and highlighted with a blue box. In the tree view on the left, 'Sample 1 (cm, 99w%, nc; 0.01h%, (Karl Fischer titration))' is selected and highlighted with a red box. A red arrow points from a yellow instruction box to this selection. A blue arrow points from another yellow instruction box to the 'Property' tab.

2. CLICK *Property*

1. SELECT the *sample* of the *compound* for which the data are to be captured.

NOTE: The **bibliographic information, compound identities, sample descriptions,** and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

Property and experimental method for squalane

Help

Property group: Critical properties

Property: Critical temperature

Units: K

Method of measurement:

Experimental purpose:

Comment (optional)

Single value Cancel

The image shows a software dialog box titled "Property and experimental method for squalane". It contains several input fields: "Property group" (set to "Critical properties"), "Property" (set to "Critical temperature"), "Units" (set to "K"), "Method of measurement", "Experimental purpose", and "Comment (optional)". At the bottom are "Single value" and "Cancel" buttons. Three callout boxes with arrows point to the "Property group", "Property", and "Units" fields, providing instructions on how to select these values from a menu.

1. SELECT the **Property Group:** *Critical Properties* from the menu.

2. SELECT the **Property:** *Critical Temperature*

3. SELECT the **Units** from the menu; *K*.

Property and experimental method for squalane

Help
Property g
Property:
Units:

Method of measurement: Other experimental method (please, describe in "Comments")

Experimental purpose: Principal objective of the work

Comment (optional) Flow Method with low residence time

Single value

Cancel

1. SELECT **Method of Measurement** from the list provided. **NOTE:** Other can be a valid selection and should include a brief description in the *Comment* field.

2. SELECT the **Experimental Purpose** from the list provided.

3. CLICK **Single value**.

1. **Phase 1** and **Phase 2** are pre-selected by GDC based on the property; T_c .

The screenshot shows a software window titled "Critical temperature as single valued property". The window contains the following elements:

- Substance:** A dropdown menu with "squalane" selected.
- Sample #:** A dropdown menu with "1" selected.
- Property set #:** A text input field containing "1".
- Phase 1:** A dropdown menu with "Liquid" selected.
- Phase 2:** A dropdown menu with "Gas" selected.
- Property value:** A text input field containing "795.9" with a unit "K" to its right.
- Precision:** A text input field containing "1".
- No of determinations:** An empty text input field.
- Comment to this record:** A text area containing "Flow Method with low residence time".
- Buttons:** "Property and method", "Accept", and "Cancel".

Four numbered instructions are overlaid on the screenshot:

1. **Phase 1** and **Phase 2** are pre-selected by GDC based on the property; T_c .
2. **ENTER** the **Property value**
3. **ENTER** the **Precision**.
4. **CLICK** *Accept*

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

NOTE: The new data set appears in the tree under the appropriate *Sample*.

[-] 2000 von wil 0

[-] squalane

[-] Sample 1 (cm,99w%,nc,;0.01h%,(Karl Fischer titration))

^0: TC(L,G,&), Set 1, B Method:OTHER

NOTE: DOUBLE CLICKING on the *data set* allows editing of all entered information.

END

**Continue with other compounds,
samples, properties, reactions, etc...**

or save your file and exit the program.